

Hamiltonian Flow Equations for the Lipkin Model

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Abstract

We derive Hamiltonian flow equations giving the evolution of the Lipkin Hamiltonian to a diagonal form using continuous unitary transformations. To close the system of flow equations, we present two different schemes. First we linearize an operator with three pairs of creation and destruction operators by reducing it to the z component of the quasi spin. We obtain the well known RPA-result in the limit of large particle number. In the second scheme we introduce a new operator which improves the resulting spectrum considerably especially for few particles.

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Recently, a new method [1, 2] has been developed in condensed matter physics to find approximate solutions in many-body theory. This method is based on flow equations for the evolution of generalized Hamiltonian couplings with a fictitious parameter ℓ running from zero to infinity. The evolution parameter ℓ characterizes the interval of energies $|E_i - E_j| < 1/\sqrt{\ell}$, for which the Hamiltonian has sizeable non-diagonal matrix elements. In the limit $\ell \rightarrow \infty$ the Hamiltonian is diagonalized. The Hamiltonian flow equations have been successfully applied to the problems of electron-phonon coupling [2], to BCS theory [3] and dissipative systems. It is natural also to try out this method on the Lipkin model [4], which is a standard test case for approximation methods in nuclear physics. The Lipkin model is exactly solvable, since its Hamiltonian is composed of bilinear products of creation and destruction operators which have a quasi-spin representation. Recently, new interest in the Lipkin model has developed in the context of finite temperatures [5] and as a test of self-consistent RPA-type approximations [6]. The Hamiltonian flow equations for the Lipkin model can be closed if one linearizes higher products of quasi-spin operators into a product of expectation values and a quasi-spin operator. When the number of particles N is very large we naturally reproduce the RPA results for $N \rightarrow \infty$. Extra care is necessary to achieve satisfactory results for mesoscopic problems with $N = (8, 10..20)$ particles. We will give an example how to improve the simple linear scheme.

In the Lipkin model N particles can distribute themselves on two levels, which are both N -fold degenerate. The splitting of the levels is ξ_0 and the interaction V_0 mixes states where two particles simultaneously move from the lower level to the higher level or vice versa:

$$\mathcal{H} = \frac{1}{2}\xi_0 \sum_{\sigma,p} \sigma a_{p\sigma}^+ a_{p\sigma} + \frac{1}{2}V_0 \sum_{pp',\sigma} a_{p\sigma}^+ a_{p'\sigma}^+ a_{p'-\sigma} a_{p-\sigma} \quad (1)$$

In the Hartree-Fock ground state all particles are in the lower level, where they have the quasi-spin $\sigma = -1$. Therefore the total quasi-spin J_z ,

$$J_z = \frac{1}{2} \sum_{p,\sigma} \sigma a_{p\sigma}^+ a_{p\sigma}, \quad (2)$$

has the value $\langle J_z \rangle = -\frac{1}{2}N$.

The interaction term can also be expressed in terms of quasi-spin operators. The Hamiltonian \mathcal{H} then has the form

$$\mathcal{H} = \xi_0 J_z + V_0 (J_+^2 + J_-^2), \quad (3)$$

where

$$J_+ = \frac{1}{\sqrt{2}} \sum_p a_{p,+1}^+ a_{p,-1}, \quad J_- = \frac{1}{\sqrt{2}} \sum_p a_{p,-1}^+ a_{p,+1}, \quad (4)$$

and J_z form an angular momentum algebra

$$\begin{aligned} [J_z, J_{\pm}] &= \pm J_{\pm}; \\ [J_+, J_-] &= J_z. \end{aligned} \quad (5)$$

Since $[\vec{J}^2, \mathcal{H}] = 0$, the interaction mixes only states in the quasi-spin multiplet $J = \frac{1}{2}N$. In the following we will consider a limited range of couplings such that the Hartree-Fock ground state remains stable, i.e. $\varepsilon = \frac{NV_0}{\xi_0} < 1$, otherwise one would have to transform to a deformed basis [6].

The concepts of unitary transformations to diagonalize the Hamiltonian is well established. Negative energy states can be eliminated from the Dirac equation by unitary transformations [7, 8]. The e^S method [9] with a suitable ansatz for the operator S has been extremely successful to derive the hierarchy of two-, three- and more-body correlations in many-particle systems, especially nuclei. The new idea in the Hamiltonian flow equations is to make the unitary transformation infinitesimal, so that it can adjust itself best to diagonalize the Hamiltonian at each stage of the flow.

In the field theory of critical phenomena it is advantageous to gradually integrate out momentum shells instead of eliminating the whole high momentum region in one step. In Hamiltonian theory the energy representation is the most useful representation for unitary transformations to eliminate non-diagonal matrix elements of shorter and shorter range. The resulting couplings in \mathcal{H} and therefore the Hamiltonian itself will then carry an index ℓ , labeling the stage of diagonalization. With $\tilde{\eta}$ anti-hermitian the unitary transformed \mathcal{H} has the following form

$$\mathcal{H}' = e^{\tilde{\eta}} \mathcal{H} e^{-\tilde{\eta}}. \quad (6)$$

In the case of an infinitesimal $\tilde{\eta} = \eta \Delta \ell$ we approximate the change

$$\mathcal{H}(\ell + \Delta \ell) - \mathcal{H}(\ell) = [\eta(\ell), \mathcal{H}(\ell)] \Delta \ell \quad (7)$$

and obtain the Hamiltonian flow equation:

$$\frac{d\mathcal{H}(\ell)}{d\ell} = [\eta(\ell), \mathcal{H}(\ell)]. \quad (8)$$

In general one chooses η proportional to the commutator of the diagonal part of the Hamiltonian \mathcal{H}_D and \mathcal{H} in order to decrease the magnitude of the off diagonal matrix elements during evolution:

$$\eta(\ell) = [\mathcal{H}_D(\ell), \mathcal{H}(\ell)]. \quad (9)$$

It is easy to follow the non-diagonal matrix elements of \mathcal{H} in the course of evolution with ℓ :

$$\frac{d\mathcal{H}_{ij}}{d\ell} = \sum_k (\eta_{ik} \mathcal{H}_{kj} - \mathcal{H}_{ik} \eta_{kj}) \quad (10)$$

and

$$\eta_{ik} = (E_i - E_k) \mathcal{H}_{ik} \quad (11)$$

gives

$$\frac{d\mathcal{H}_{ij}}{d\ell} = -(E_i - E_j)^2 \mathcal{H}_{ij} + \mathcal{O}((\mathcal{H}_{ij})^2). \quad (12)$$

The leading term in eq. (12) arises by using the diagonal part of the Hamiltonian in eq. (10). The off-diagonal part of the Hamiltonian yields sub-leading terms. The resulting equation suggests a damping of the non-diagonal elements which decrease with increasing ℓ .

Let us first take the original Hamiltonian with ℓ -dependent couplings and study its evolution with the Hamiltonian flow equations. We improve the scheme in the second half of the paper by adding a term which starts out as zero for $\ell = 0$ but grows during the evolution. The generalized Hamiltonian $\mathcal{H}(\ell)$, together with the initial conditions, has the following form:

$$\begin{aligned}\mathcal{H}(\ell) &= \xi(\ell)J_z + V(\ell)(J_+^2 + J_-^2), \\ \xi(0) &= \xi_0, \\ V(0) &= V_0.\end{aligned}\tag{13}$$

Defining η as $\eta = [\mathcal{H}_D, \mathcal{H}]$ with $\mathcal{H}_D = \xi(\ell)J_z$ we obtain:

$$\eta = 2\xi V(J_+^2 - J_-^2).\tag{14}$$

By inserting this η into the flow equation we find:

$$\begin{aligned}\frac{d\mathcal{H}}{d\ell} &= [\eta, \mathcal{H}] \\ &= 4\xi V^2(2J_z(\bar{J}^2 - J_z^2) - J_z) - 4\xi^2 V(J_+^2 + J_-^2).\end{aligned}\tag{15}$$

The right hand side of this equation contains an hermitian operator containing three quasi spins $\propto J_z^3$, i.e. a term different from the original evolving Hamiltonian (13). This new term is approximated by linearizing around the Hartree-Fock operator expectation values:

$$AB = (A - \langle A \rangle)(B - \langle B \rangle) - \langle A \rangle \langle B \rangle + \langle A \rangle B + A \langle B \rangle\tag{16}$$

which yields:

$$J_z^3 \rightarrow 3\langle J_z \rangle^2 J_z.\tag{17}$$

A linearization of J_z^3 is certainly meaningful when the fluctuations of J_z around its expectation value are small, i. e. for large quasi spins. This is the case for the lowest lying levels, if the particle number is large.

Differentiation of the ansatz for $\mathcal{H}(\ell)$ in eq. (13) gives the left side of the evolution equation

$$\frac{d\mathcal{H}}{d\ell} = \frac{d\xi}{d\ell} J_z + \frac{dV}{d\ell} (J_+^2 + J_-^2)\tag{18}$$

which we compare with the approximate result for the commutator from eq. (15).

We see that the ansatz for $\mathcal{H}(\ell)$ in eq. (13) together with the approximation for the cubic operator product indeed leads to a closed system of first order differential equations for the coefficients in front of the quasi-spin operators.

$$\begin{aligned}\frac{d\xi}{d\ell} &= -4\xi V^2[N(N-1) + 1], \\ \frac{dV}{d\ell} &= -4\xi^2 V.\end{aligned}\tag{19}$$

The second equation implies that the magnitude of the off-diagonal matrix element V decreases in the course of the evolution, independently of its sign. Combining the two equations one readily obtains an invariant of the evolution:

$$\xi^2(\ell) - [N(N-1) + 1]V^2(\ell) = \xi_0^2 - [N(N-1) + 1]V_0^2. \quad (20)$$

Using $V(\infty) = 0$ one finds the limiting value of ξ and the splitting Δ between the ground state and first excited state :

$$\begin{aligned} \xi(\infty) &= \xi_0 \sqrt{1 - \bar{\varepsilon}^2}, \\ \bar{\varepsilon} &= \sqrt{N(N-1) + 1} \frac{V_0}{\xi_0}; \\ \Delta &= \langle 1 | \mathcal{H}(\infty) | 1 \rangle - \langle 0 | \mathcal{H}(\infty) | 0 \rangle \\ &= \xi(\infty). \end{aligned} \quad (21)$$

In the large N -limit with finite interaction strength the splitting Δ between the ground state and first excited state has the form of the RPA approximation [4]

$$\begin{aligned} \Delta_{RPA} &= \xi_0 \sqrt{1 - \varepsilon^2}, \\ \varepsilon &= N \frac{V_0}{\xi_0}. \end{aligned} \quad (22)$$

In nuclear physics one studies systems with intermediate particle number. Neither few nor many body methods are directly applicable. In nuclei the relevant number of particles is given by the number of particles outside of closed shells, which is $N \leq 2J + 1$, where J is the angular momentum of the valence shell. We want to obtain a reliable result also for small values of N . To this end we propose to add a new operator to the original Hamiltonian, which improves the accuracy of the evolution equations. The new term $\propto J_z^3$ has been chosen to have the same symmetry as the original Hamiltonian under reflections. From the previous flow equations such an improvement is suggested, since a term $\propto J_z^3$ was generated on the right hand side of the previous evolution equation (15). Adding new operators generated from the original Hamiltonian by the commutators is an established way to improve the method. Obviously symmetry provides an important guideline for the choice of new operators to be included in the Hamiltonian $\mathcal{H}(\ell)$. Usually the commutators generate additional terms which must be eliminated, since one can obtain a closed set of differential equations only if every operator on the right side of the evolution equation has a counterpart on the left-hand side of eq. (8). We choose:

$$\mathcal{H}(\ell) = \xi(\ell)J_z + V(\ell)(J_+^2 + J_-^2) + \gamma(\ell)J_z^3 \quad (23)$$

with the initial conditions

$$\xi(0) = \xi_0; \quad V(0) = V_0; \quad \gamma(0) = 0. \quad (24)$$

Proceeding along similar lines as before we define η as

$$\eta = [\xi J_z, \mathcal{H}] \quad (25)$$

slightly deviating from the commutator of $[\mathcal{H}_D, \mathcal{H}]$. Otherwise terms with higher powers of quasi spins would be produced. The explicit calculation of η leads to the same anti-hermitian operator product as before.

$$\eta = 2\xi V(J_+^2 - J_-^2). \quad (26)$$

Inserting this η into the flow equation we get

$$\frac{d\mathcal{H}}{d\ell} = 4\xi V^2(2J_z(\vec{J}^2 - J_z^2) - J_z) - 4\xi^2 V(J_+^2 + J_-^2) + 2\xi V\gamma[(J_+^2 - J_-^2), J_z^3]. \quad (27)$$

We see a new operator product appearing from the commutator of η with the γ term in \mathcal{H} . Using the reduction scheme for products of operators described above, we find

$$[(J_+^2 - J_-^2), J_z^3] \rightarrow -6\langle J_z \rangle^2(J_+^2 + J_-^2) \quad (28)$$

This way we regain a closed system of first order evolution equations for the coefficients in front of the quasi-spin operators

$$\begin{aligned} \frac{d\xi}{d\ell} &= 4\xi V^2[2J(J+1) - 1], \\ \frac{dV}{d\ell} &= -4\xi^2 V - 12\xi V\gamma\langle J_z \rangle^2, \\ \frac{d\gamma}{d\ell} &= -8\xi V^2. \end{aligned} \quad (29)$$

We introduce the abbreviations

$$\begin{aligned} r &= 2\vec{J}^2 - 1 = 2J(J+1) - 1, \\ s &= \frac{3}{4}\langle J_z \rangle^2, \\ t &= \frac{8s}{r}. \end{aligned} \quad (30)$$

Combining the first and third evolution equation we find the invariant

$$\frac{\xi}{r} + \frac{\gamma}{2} = \frac{\xi_0}{r}, \quad (31)$$

where we employ the initial conditions on the right hand side. By using this relation we eliminate γ as independent variable. A second more complicated invariant arises from all three equations and has the form

$$\xi^2 + rV^2 - t(\xi_0 - \xi)^2 = \xi_0^2 + rV_0^2. \quad (32)$$

The allowed values of ξ and V lie on a hyperbola as shown in fig. 1. For the plot we choose $\varepsilon = 0.8$ and $t = 3$, which is approximately true for large N . At the beginning of the evolution at $\ell = 0$ we start on the hyperbola at $\xi = \xi_0$ and $V = V_0$. Since the gradient $d\xi/d\ell > 0$ the magnitude of ξ is growing and V decreases. Thus the point

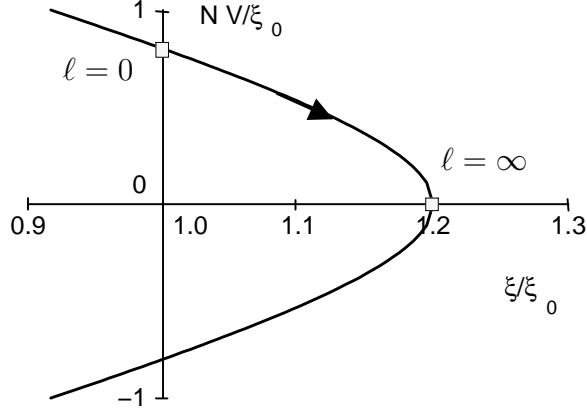


Figure 1: Flow in the $\xi - V$ plane as defined by eqs. (29) and (32)

$V = 0$, where the right hand sides of all three evolution equations vanish, is a stable fix point. The variables ξ and γ converge towards the fix point values

$$\xi(\infty) = \frac{\xi_0}{t-1} \left[t - \sqrt{1 - 3 \left(\frac{t-1}{2t} \right) \varepsilon^2} \right], \quad (33)$$

$$\gamma(\infty) = \frac{2\xi_0}{r(t-1)} \left[-1 + \sqrt{1 - 3 \left(\frac{t-1}{2t} \right) \varepsilon^2} \right]. \quad (34)$$

The above expressions depend on the particle number N through the constants r, s, t in a rather complicated way. Due to the presence of the J_z^3 term in the Hamiltonian the splitting Δ between the ground state and first excited state has the modified form:

$$\begin{aligned} \Delta &= \langle 1 | \mathcal{H}(\infty) | 1 \rangle - \langle 0 | \mathcal{H}(\infty) | 0 \rangle \\ &= \xi(\infty) + \gamma(\infty) \left(\frac{3N^2}{4} - \frac{3N}{2} + 1 \right) \end{aligned} \quad (35)$$

In fig.2 we show the energy gap Δ for three different interaction strengths $\varepsilon = 0.4, 0.6, 0.8$. The curves with stars are the result of an exact diagonalization of the Hamiltonian. The full drawn curves give the improved result from the evolution equations (29). For comparison we also show the result of the evolution equations (19) with long dashes and the RPA result (22) with short dashes. One sees that the method is very accurate for weak interactions, where perturbation theory also does a rather good job. In the case of strong coupling there are still some deviations for intermediate particle numbers. The larger the coupling the closer one is to the transition to a deformed ground state, therefore also the fluctuations become

stronger and our expansion of the new operators in powers of fluctuating operators is not so good anymore. All three calculations approach the RPA result for large particle numbers shown with short dashes. In the limit of large N one can also demonstrate analytically that the improved method converges to the RPA result.

Applying the evolution equations to the Lipkin model one encounters the problem that ever new operators are generated in the course of setting up the evolution equations. This is a general feature of spin models. Similar features occur in the spin boson problem. The original Lipkin Hamiltonian has a rather simple tridiagonal structure, which is lost during the evolution for finite ℓ , if one does not enforce it by suitable approximations. Recently Mielke [10] has constructed an η -operator which preserves the simple structure of the Lipkin Hamiltonian without approximations, but still reduces the magnitude of the off-diagonal matrix elements. This method is also applicable beyond the stability of the Hartree-Fock state ($\varepsilon > 1$).

In conclusion, we have set up Hamiltonian flow equations for the Lipkin model. By infinitesimal unitary transformation we have diagonalized the Hamiltonian approximately making reasonable truncations for the new operators. We have presented an improved scheme which successfully interpolates between perturbation theory for small N and RPA for large N . The method of evolution equations has been shown to be a promising new tool also for nuclear physics. It opens up new perspectives for approximations in many body problems which still have to be explored in greater detail. Thus a systematic approach to select the relevant set of operators for the evolution equations can be established.

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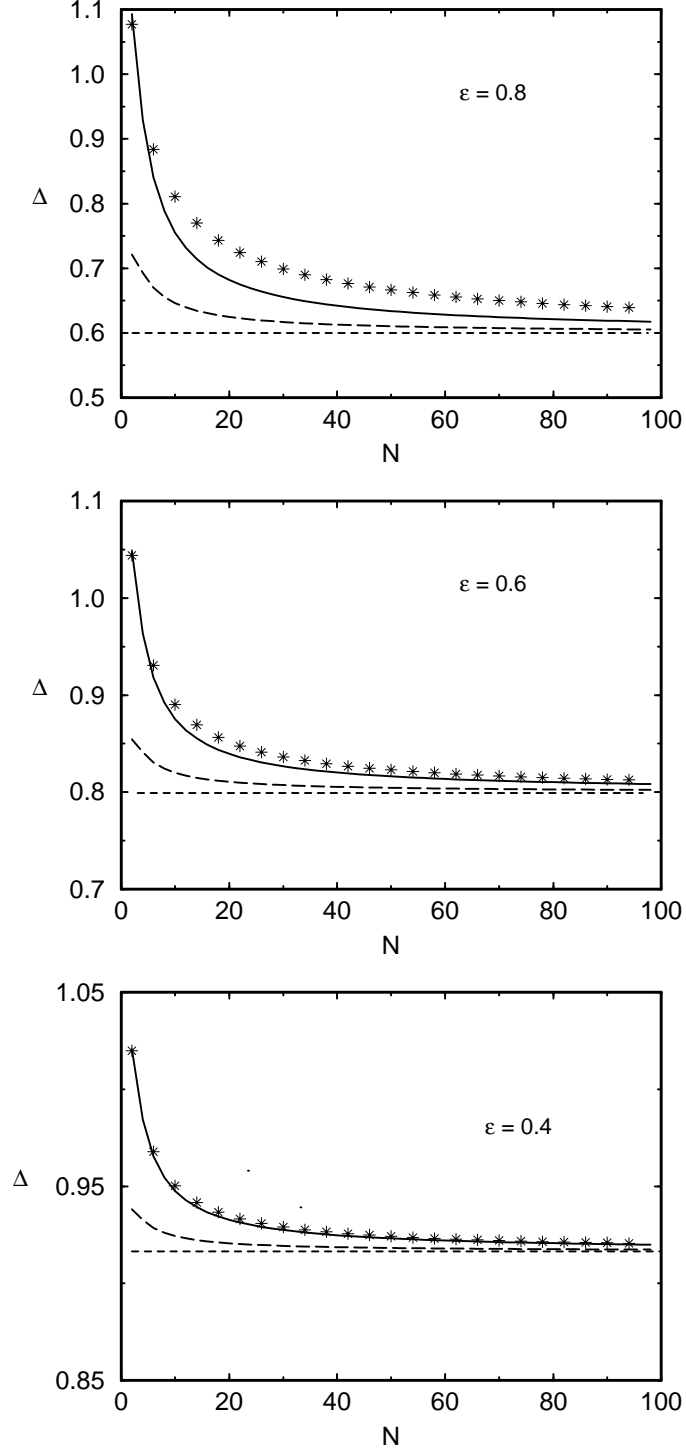


Figure 2: Energy gap Δ between ground state and first excited state for various strengths $\varepsilon = 0.4, 0.6, 0.8$. Stars denote the exact result, solid line shows the improved result from the evolution equations, while the long-dashed line gives the result of the linearized scheme. The short-dashed line is the RPA result.